Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -3.32 °C

Global applicability domain: Inside

Local applicability domain index: 1.00

Confidence level: 4.97e-01

Nearest Neighbors from the Training Set

Image not found
Cyclopentane
Measured: -93.8
Predicted: -3.32

Image not found
Cycloheptane
Measured: -8.00
Predicted: -3.32

Image not found
Cyclooctane
Measured: 14.8
Predicted: -3.32

Image not found
Cyclodecane
Measured: 10.0
Predicted: -33.5

Image not found
Cyclododecane
Measured: 60.4
Predicted: -3.32